Asulam

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 152 °C

Global applicability domain: Inside

Local applicability domain index: 4.15e-01

Confidence level: 6.42e-01

Nearest Neighbors from the Training Set

Image not found
Asulam
Measured: 144
Predicted: 152

Image not found
Sulfacetamide
Measured: 183
Predicted: 189

Image not found
4'-Sulfamylacetanilide
Measured: 220
Predicted: 205

Image not found
Sulfadicramide [INN:DCF]
Measured: 185
Predicted: 190

Image not found
Felbamate
Measured: 152
Predicted: 150